

Gate errors in solid state quantum computation

Xuedong Hu and S. Das Sarma

Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD 20742-4111

We review our work on the interplay between non-resonant gates and solid state environment in various solid state quantum computer architectures and the resulting gate errors. Particular, we show that adiabatic condition can be satisfied in small quantum dots, while higher energy excited states can play important role in the evolution of a Cooper-pair-box based quantum computer model. We also show that complicated bandstructure such as that of Si can pose a severe gate control problem.

I. INTRODUCTION

It has been pointed out for a long time that quantum mechanics may provide great advantages over classical physics in physical computation [1,2]. The recent rapid growth of research on quantum computation [3] started after Shor's factorization algorithm [4] and quantum error correction codes [5,6] were developed. For a quantum system to be used as a quantum computer (QC), it has to satisfy some stringent conditions [7]. In short, it should possess a scalable Hilbert space; the state of such a system should be easily initialized; the system should have a long decoherence time; there should be a set of universal unitary gates applicable to the system; and last but not least, every single quantum bit (qubit) of the system should be faithfully measured. Here we would like to review our work on the quantum gates and their operations in various solid state quantum computer architectures.

Many two-level systems have been proposed as candidates for qubits in a solid state quantum computer. Typical examples include electron spins, nuclear spins, electron charge states, Cooper pair charge states, superconducting flux states, and many more [8–14]. One major motivation for these solid state devices is their potential in scalability. However, solid state structures also present complex environments and fast decoherence rates [15]. Furthermore, in most solid state QC schemes, non-resonant gate operations [8,11,13,16] are crucial or important components. It is thus necessary to understand how the environmental elements affect the QC coherent evolution, and clarify the effects of imperfections in non-resonant gate operations. In the following, we will review some of the results we have obtained for three different quantum computer architectures: the spin-based quantum dot QC, the Cooper-pair-box-based QC, and the donor-nuclear-spin-based Si QC.

II. NON-ADIABATIC OPERATIONS IN A DOUBLE QUANTUM DOT

Let us first discuss our work on the spin-based quantum dot quantum computer (QDQC) in GaAs [8,9]. Here two-qubit operation is based on the nearest neighbor exchange coupling, which produce the exchange splitting

between the ground singlet and triplet states. For small quantum dots, with large single particle excitation energy E_s and large on-site Coulomb repulsion energy E_C and at low temperatures ($k_B T \ll \min\{E_s, E_C\}$), the low energy dynamics is dominated by the electron spins. In other words, one can focus on the spin part of the two-electron Hilbert space that involves only the ground singlet and triplet states and cut off the rest of the Hilbert space. For example, at $T \sim 100$ mK and with $\min\{E_s, E_C\} \sim 1$ meV, the thermal occupation of the higher energy orbital states is less than 10^{-50} , which can be safely neglected. Thus one can quite faithfully prepare a single electron in a single dot in its ground orbital state and/or two electrons in a double dot in the ground singlet/triplet state manifold. For a double dot, after the state is initialized, as long as the applied quantum gates satisfy adiabatic condition, the system would remain in the ground state manifold, so that Heisenberg exchange Hamiltonian would describe the dynamics of the double quantum dot exactly. However, the size of a gated quantum dot is limited from below by gate and device dimensions, while the gate operating time is limited from above by the electron spin decoherence time. Thus it is necessary to quantitatively assess the adiabatic condition for two-qubit operations in a double dot of realistic dimensions, so as to determine whether exchange gates can be sufficiently fast to guarantee a large gate-time/decoherence-time ratio while slow enough to produce correctly small non-adiabatic errors.

We have performed a quantitative evaluation of the adiabatic condition in a double quantum dot [17] using the results of our molecular orbital calculation of the double energy spectra [9]. Specifically, we prepare a two-electron state in the ground singlet state with a high barrier between the double dot. As the system evolves, the barrier height between the two dots is first lowered, then raised back to the original value. If Heisenberg exchange Hamiltonian is exact for this system, its state should remain in the ground singlet state. Any loss from this state would then constitute a leakage from the QC Hilbert space and a gate error.

Our calculation is essentially an integration of the time-dependent Schrödinger equation for the two-electron double quantum dot:

$$\frac{\partial c_k(t)}{\partial t} = \sum_{i \neq k}^N \frac{c_i(t)}{E_k(t) - E_i(t)} \langle k | \frac{\partial H(t)}{\partial t} | i \rangle \times \exp \left\{ \frac{1}{i\hbar} \int_{-\infty}^t (E_i(\tau) - E_k(\tau)) d\tau \right\}. \quad (1)$$

Here $c_k(t)$ are the coefficients as we expand the two-electron state on the instantaneous eigenstates $|k\rangle$: $\psi(t) = \sum_k c_k(t) u_k(t)$ and $H(t)u_k(t) = E_k(t)u_k(t)$, where $H(t)$ is the time-dependent system Hamiltonian. The explicit time-dependence of H is in the inter-dot barrier height. Since initially the system is entirely in the ground singlet state, $c_k(t=0) = \delta_{k0}$ for all k . The energy spectra we use are for a double dot with Gaussian confinements of 30 nm radii and 40 nm inter-dot distance [9]. The energy barrier height V_b ranges between 14 meV and 35 meV, corresponding to exchange splitting of 280 μ eV to 3.3 μ eV. By varying the barrier variation time, we can quantitatively evaluate the change in the ground singlet state population, thus obtaining a lower limit to the gate operating time using the criterion of quantum error correction code threshold.

The result of our calculation is plotted in Fig. 1 [17]. The leakage (y-axis) is defined as $1 - |c_0|^2$ which is zero before the gate is applied, and should be zero if the gate is perfectly adiabatic. Aside from several interesting features [17], Fig. 1 demonstrates that for gating time longer than 30 \sim 40 ps, leakage in our double dot system should be sufficiently small ($\lesssim 10^{-6}$) so that the currently available quantum error correction schemes would be effective. On the other hand, an exchange splitting of 0.1 meV corresponds to about 20 ps gating time for a swap gate [8] (with rectangular pulse) at the shortest. Therefore, adiabatic condition does not place an extra burden on the operation of the two-qubit gates such as a swap—there is in general no need to significantly increase the gating time in order to accommodate the adiabatic requirement.

Notice that the current calculation is done for a pair of quite small quantum dots. Larger dots would have meant smaller excitation energies and a threshold gating time that is longer in order to satisfy the adiabatic condition.

III. NON-SUDDEN OPERATIONS IN A COOPER PAIR BOX

Another example we have considered is the Cooper pair box quantum computer (CPBQC) [17]. The Hamiltonian of a Cooper pair box (CPB) can be written on the basis of charge number states of the box:

$$\begin{aligned} H &= 4E_C(\hat{n} - n_g)^2 - E_J \cos \hat{\phi} \\ &= \sum_n [4E_C(n - n_g)^2 |n\rangle\langle n| \\ &\quad - \frac{E_J}{2} (|n\rangle\langle n+1| + |n+1\rangle\langle n|)], \end{aligned} \quad (2)$$

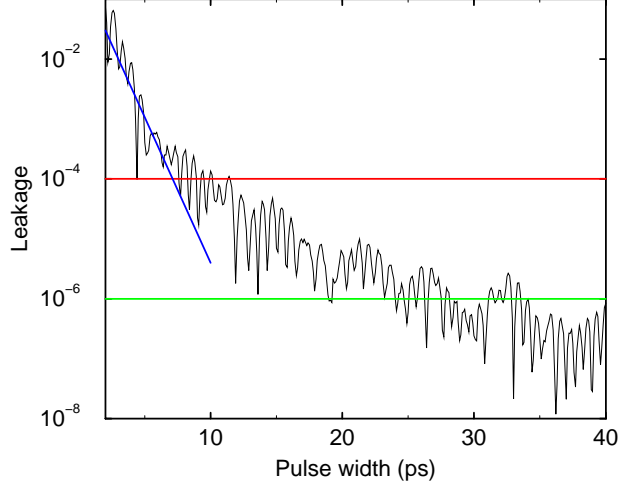


FIG. 1. Leakage as a function of the pulse width 2τ of the exchange gate. The two-electron state is initially in the ground singlet state. The two horizontal lines represent the commonly used thresholds for quantum error correction. The fitted line at the small pulse-width indicates the initial rapid decrease in the error rate (leakage) as the pulse becomes wider (or the gate operation becomes slower).

where E_C is the charging energy of a CPB, E_J is the Josephson coupling between the CPB and an external superconducting lead, n_g represents the applied voltage on the CPB in terms of an effective charge number, and n refers to the number of extra Cooper pairs in the box. Due to the periodic nature of the Josephson coupling, the eigenstates of a CPB form energy bands. The two states $|\uparrow\rangle$ and $|\downarrow\rangle$ for a CPB qubit correspond to the two lowest energy levels at $n_g = 1/2$, where the eigenstates are approximately $|\downarrow\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ and $|\uparrow\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$ with a splitting of about E_J .

Similar to the case of QDQC discussed above, higher excited states play an important role in the dynamics of a CPBQC when it is subjected to non-resonant operations [18]. The particular operation we considered is the sudden pulse gate to shift n_g , thus bringing a system from a pure ground state $|0\rangle$ at, e.g. $n_g = 1/4$ to a coherent superpositioned state $(|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$ at $n_g = 1/2$. Such a simple description of the pulse gate is only valid when $E_J/E_C \rightarrow 0$. Since E_J determines the gate speed of a CPBQC, such a condition is not practical for a realistic QC. Furthermore, in real experiments, the pulse gate always has finite rise/fall times (non-sudden). In Ref. [16], the pulse rise time is in the range of 30 to 40 ps. Such gradual rise and fall of the pulse gate inevitably lead to more errors, which have been considered in the context of two-level systems [16,19,20]. What we have done is to calculate the fidelity of the pulse gate taking into account the finite rise/fall time, the higher excited states, and the complete composition of all the eigenstates [17].

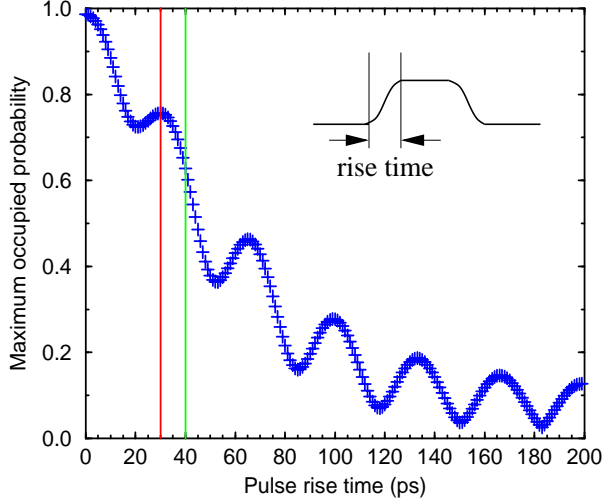


FIG. 2. State fidelity as a function of the finite rise/fall time of a pulse gate in a single Cooper pair box. The fidelity here is defined as the maximum probability (which implies particular choices of pulse duration τ_p as this probability varies periodically with τ_p) of the CPB in the first excited state after the application of a pulse gate with the state starting from the ground state (represented by n_g goes from 0.255 to 0.5, then back to 0.255 after a period of time τ_p). The CPB is treated as a multi-level system (on the basis of $|-10\rangle, \dots, |0\rangle, |1\rangle, \dots, |10\rangle$). The lineshape of the rise/fall of the pulse is a sinusoidal function of time. The system parameters are chosen as the values used in Ref. [16]. The two vertical lines give the range of rise/fall time from the same source.

In Fig. 2 we plot the state fidelity as a function of rise time. Here the state fidelity is defined as the maximum probability for the CPB to be in the first excited state after the pulse gate when n_g returns to 0.255. Figure 2 shows that the fidelity of the pulse gate decreases oscillatorily instead of monotonically as the pulse rise time increases. The oscillations (with periods around 30 ps) in the curves represent the coherent evolution of the CPB during the rise/fall of the pulse voltage. For pulses used in Ref. [16] with rise/fall time in the range of 30 to 40 ps, the fidelity is only 60 to 70 %, apparently not sufficient for manipulations required by quantum computation. Further calculations also demonstrate that including higher excited states is important in correctly evaluating the fidelity dependence on the rise time of the non-resonant sudden pulse gate [17].

IV. IMPLICATIONS OF SI BANDSTRUCTURE

The previous two examples demonstrate the interplay of non-resonant gate operations and states from the full Hilbert space, and the resulting leakage from the computational space. Solid state environment can affect the

operation of a quantum computer in other subtle ways. For example, modern technology can produce extremely pure silicon crystals which have the intrinsic property of very small spin-orbit coupling. Thus electron and nuclear spins in Si have a very “quiet” environment—the spin relaxation times are extremely long in Si [21,22]. It is therefore natural to use Si as a host material for spin-based quantum computer architectures [11]. However, Si is an indirect gap semiconductor. There are actually six equivalent minima in its conduction band that are away from the center of the First Brillouin zone and close to the zone boundary. The implication of this complexity is that confined electron states (whether the confinement is provided by a donor or a gate-produced electrostatic potential in the form of a quantum dot) in general have contributing components from all the valleys, which can then lead to atomic scale spatial oscillations of electronic properties such as electron density and two-electron exchange coupling.

We have performed a Heitler-London calculation for the two-electron exchange splitting for two phosphorus donors in Si [23]. The Si:P system is being studied as a candidate of nuclear spin based quantum computers [11,24]. Donor electron exchange is a crucial intermediary in the effective nuclear spin exchange interaction that is the basis of the two-qubit operations in such a quantum

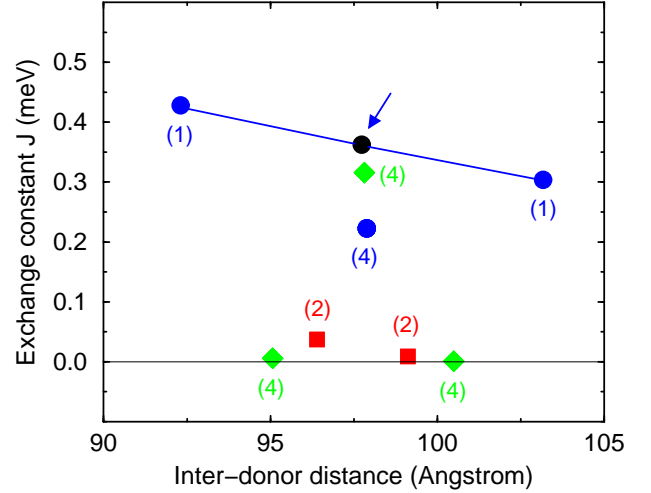


FIG. 3. Variations in the exchange coupling between two phosphorus donors in Si. The arrow points at the circle that represents the value of electron exchange at the reference configuration with the two donors exactly along the [100] direction and separated by 18 lattice constants. The circles connected by a line refer to pairs along the [100] direction, displaced by one lattice constant with respect to the reference position. The rest of the symbols represent displacements of one member of the donor pair into one of its first (squares), second (diamonds), or third (circles) nearest neighbor positions. The numbers in the parenthesis next to the symbols are their degeneracies, respectively.

computer architecture. Our calculation indeed shows a fast-varying exchange, as is demonstrated in Fig. 3, which shows that a movement of one member of the donor pair into its nearest or second nearest neighbor sites can completely suppress the exchange coupling between the two donor electrons.

In the original proposal of Si quantum computer [11], electron exchange is tuned by applied gate voltages, which would shift the electron wavefunctions. Thus the two-qubit gates here are exposed to the atomic-scale oscillations. The direct implication of the oscillatory exchange is that the gate voltages corresponding to the peak exchange coupling have to be well-controlled, optimally close to a local maximum where the exchange is least sensitive to the gate voltage. Since the oscillatory exchange period is close to lattice spacing, the positioning of the donor electrons by the surface gates must be controlled at least to that precision.

V. ACKNOWLEDGMENT

We thank financial support from ARDA and LPS and collaborations (on the donor exchange in Si) and helpful discussions with Belita Koiller.

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